Improved modeling of Coulomb effects in nanoscale Schottky-barrier FETs

Klaus Michael Indlekofer, Joachim Knoch, and Joerg Appenzeller

***Abstract*— We employ a novel multi-configurational self-consistent Green's function approach (MCSCG) for the simulation of nanoscale Schottky-barrier field-effect transistors. This approach allows to calculate the electronic transport with a seamless transition from the single-electron regime to room temperature field-effect transistor operation. The particular improvement of the MCSCG stems from a division of the channel system into a small subsystem of resonantly trapped states for which a many-body Fock space becomes feasible and a strongly coupled rest which can be treated adequately on a conventional mean-field level. The Fock space description allows for the calculation of few-electron Coulomb charging effects beyond mean-field.**

We compare a conventional Hartree non-equilibrium Green's function calculation with the results of the MCSCG approach. Using the MCSCG method Coulomb blockade effects are demonstrated at low temperatures while under strong nonequilibrium and room temperature conditions the Hartree approximation is retained.

***Index Terms*— Coulomb interaction, nanowire, Schottky-Barrier FET.**

I. Introduction

ONE of the major challenges for the simulation of nanoscale field-effect transistors (FET) consists in an adequate description of the Coulomb interaction within the transistor channel: a proper simulation approach has to account for the Coulomb interaction of a few fluctuating electrons and at the same time has to be able to describe non-equilibrium transport in an open nanosystem.

For the correct many-body description of the Coulomb interaction with the inclusion of contact coupling and nonequilibrium injection conditions, Fock space approaches such as realtime renormalization group [1], [2] or the Fock space Green's function [3] are available. This class of methods provides kinetic equations in Fock space, taking renormalization and dissipation due to the coupling to the contacts (at least to some extent) and the Coulomb interaction into account. Since these approaches involve the 2^N-dimensional Fock space for the considered single-particle basis of N states, they typically are restricted to $N \lesssim 10$ for practical reasons. In the limit of small coupling, the Fock space description of the system can be approximated by a reduction to rate equations [4], [5], which deal with many-body eigenstates of the uncoupled Hamiltonian obtained via exact diagonalization [6], [7], [8], [9], containing a full description of the Coulomb interaction.

Realistic modeling of a 1D semiconductor nanotransistor typically involves a number N of single-particle states (orbital or sites) of up to a few hundred, rendering a full numerical Fock space description impossible due to the exponential scaling of the resulting many-body space dimensions. Furthermore, most of the potentially current-carrying single-particle states are stronlgy coupled to the contacts, and thus, the picture of a weakly coupled system in general becomes inadequate. The nonequilibrium Green's function (NEGF) approach [10], [11], [17], [18] in a mean-field approximation provides reasonble scalability, however, in principle lacks the description of few-electron Coulomb charging effects which become apparent in the case of resonantly trapped states in particular at lower temperatures. A possible solution is the combination of the numerically well scaling mean-field NEGF with a Fock space description for those states where many-body Coulomb effects may become important for the device characteristics. In this context, we have recently proposed a multi-configurational selfconsistent Green's function approach (MCSCG) [9], [12] for the realistic simulation of nanodevice systems under application-relevant conditions with reasonable numerical efforts.

In the following sections, we will outline the main ideas and the algorithm behind the MCSCG and demonstrate its strengths by comparing a conventional Hartree NEGF calculation with the results of the MCSCG approach, providing significantly extended information to our recent conference contribution [13]. Using the MCSCG, Coulomb blockade effects are demonstrated at low temperatures while under strong nonequilibrium and room temperature conditions the Hartree approximation is retained.

II. Multi-configurational approach

In order to handle systems with a large number N of single-particle states, the main idea of the MCSCG is to divide the system into two subsystems: Resonantly trapped (i.e. weakly coupled) states and those states that couple strongly to the contacts as depicted in Fig. 1. Within the subspace of $N' \lesssim 10$ resonantly trapped states, which require a many-body description of the Coulomb interaction, a Fock space method will be applied, whereas the rest ($N-N'$) is treated adequately on an approximated NEGF level. The eigenstates $\{|\kappa\rangle\}$ of the many-body statistical operator (or Hamiltonian, depending on the Fock space method) within the resonantly trapped subspace will be referred to as configurations with weights

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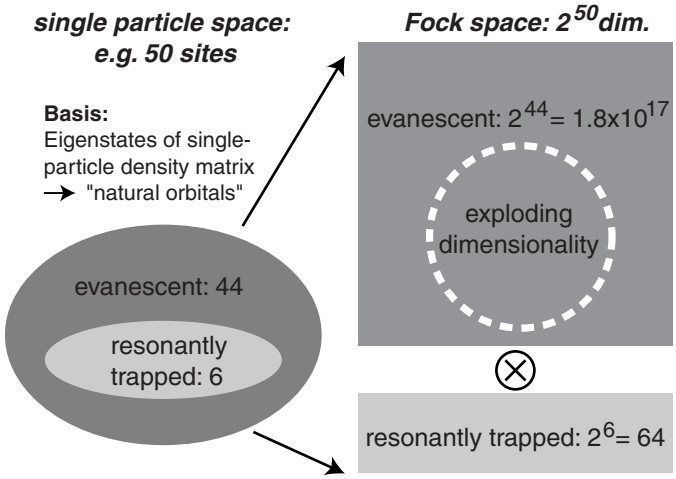

Fig. 1. Example for the division of the single-particle space into two subspaces. Only for resonantly trapped states (6 in the example), a Fock space description is employed. The rest (evanescent) is treated by a mean-field description.

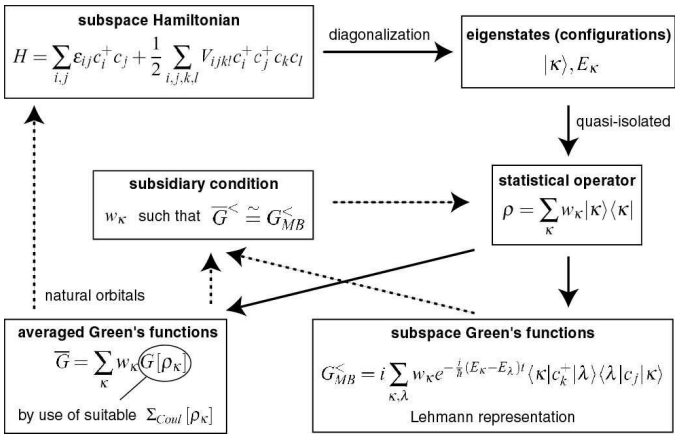

Fig. 2. Flowchart of the MCSCG algorithm. In the shown case, exact diagonalization is employed as the simplest Fock subspace method. Arrows visualize the flow of the selfconsistency loop.

$\{w_\kappa\}$ corresponding to the respective eigenvalues. Thus, the configurations and their weights follow from a Fock space calculation, taking the detailed Coulomb interaction within this subspace into account. The many-body statistical operator ρ of the considered system can be written in the general form

$$\rho = \sum_\kappa w_\kappa P_\kappa \otimes \rho_{rest}[\kappa], \tag{1}$$

where $P_\kappa \equiv |\kappa\rangle\langle\kappa|$ denotes the projection operator corresponding to the eigenstate $|\kappa\rangle$, and ρ_{rest} is the many-body statistical operator of the rest, which may depend on the configuration κ. Motivated by this form, we define a configuration-averaged Green's function $\bar{G}$ of the system as

$$\bar{G} = \sum_\kappa w_\kappa G[\kappa], \tag{2}$$

where $G[\kappa]$ corresponds to $P_\kappa \otimes \rho_{rest}[\kappa]$ and shall fulfill Dyson's equation with a suitable contact coupling plus Coulomb selfenergy approximation $\Sigma[\kappa]$. In the simplest case, $\Sigma[\kappa]$ may be of a decoupled mean-field form [9], which is adequate for temperatures well above the corresponding Kondo temperature.

As for the Fock subspace of the resonantly trapped states, the projected many-body Hamiltonian contains the reduced single-particle and Coulomb terms. Furthermore, coupling to the contacts with nonequilibrium carrier injection and coupling (tunneling) to the rest of the system is described by means of selfenergy kernels, depending on the chosen Fock space method. For the latter, various choices are possible, for example: Exact diagonaliztion with Dyson's equation as subsidiary condition [9], [12], real-time renormalization group (RTRG) [1], [2] or Fock space Green's functions [3]. In the following, we will discuss the first option, based on exact diagonalization. In this case, the many-body statistical operator is assumed to be diagonal in the eigenbasis of the resonant subspace Hamiltonian. Here, the eigenvalues w_κ are determined such that the resulting many-body Green's function G_{MB} in Lehmann representation fulfills Dyson's equation within the resonant subspace. In the simplest implementation, $\{w_\kappa\}$ is chosen such that the spectral peaks of $G^<_{MB}$ match those of $\bar{G}^<$ [9].

As an overall selfconsistency condition, the resonantly trapped states experience a mean-field interaction of the rest, whereas the rest is subject to the set $\{\Sigma[\kappa]\}$ of selfenergies originating from the resonant many-body configurations κ and its own mean-field interaction. Finally, for the identification of resonantly trapped states, the single-particle eigenstates of the single-particle density-matrix are employed (so-called natural orbitals). The latter follows directly from the Green's function $\bar{G}^<$ as part of the multi-configurational selfconsistency procedure. (Note that each individual $G[\kappa]$ need not be selfconsistent with its respective $\Sigma[\kappa]$.) In turn, resonantly trapped states are defined as those single-particle eigenstates that exhibit a level broadening (determined from the selfenergies) below a given threshold. Fig. 2 illustrates the details of the algorithm as a flowchart.

For the calculation of expectation values of single-particle observables (e.g., electron density, current, spin density, etc.), the selfconsistent Green's function $\bar{G}^<$ is employed as an approximation for the unknown exact $G^<$. Optionally, within the resonant subspace, one can use the many-body result (such as G_{MB}, the reduced statistical operator, dissipation kernel, etc.) for the evaluation of arbitrary expectation values, in particular contour-ordered correlation functions of arbitrary order.

III. Simulation of Nanoscale Schottky-barrier FETs

In order to demonstrate the strengths of the MCSCG approach, we consider a one-dimensional (1D) coaxially gated nanowire transistor with Schottky-barrier source and drain contacts since deviations from a mean-field approximation become most apparent in a system with quasi-bound states. Fig. 3 shows a schematics of such a nanowire transistor where we assume a channel length of $L = 20$nm, a diameter of

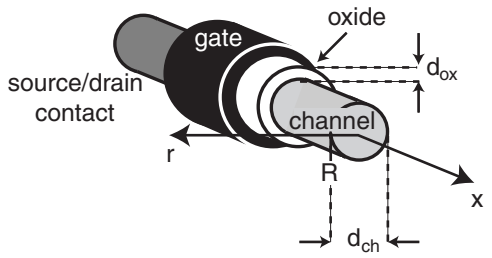

Fig. 3. Schematic sketch of a nanowire MOSFET with coaxial gate.

$d_{\rm ch} = 4$nm and a gate oxide thickness of $d_{\rm ox} = 10$nm. (Since the spin degree of freedom is included and a site spacing of $a = 1$nm is employed, we thus consider $N = 40$ single-particle states.) Such a nanowire transistor can in principle be realized with a semiconducting InGaAs nanowire with SiO_2 as gate dielectric. It has been shown that the electrostatics of coaxially gated nanowire transistors can be well described by a modified one-dimensional Poisson equation [16]. This Poisson equation allows to easily calculate the Coulomb Green's function which in turn enables the description of the classical electrostatics and the screened interaction between electrons on equal footing [9]. For the following simulation results, the simplest MCSCG variant has been employed, based on exact diagonalization (with $N' = 6$ resonantly trapped states yielding 64 Fock space dimensions) with a decoupled static selfenergy form.

Fig. 4 visualizes the simulated drain current $I_{\rm D}$ for the single-electron transport regime ($T = 77$K) as a color plot. In contrast to the Hartree-only calculation (Fig. 4(a)), the MCSCG approach (Fig. 4(b)) correctly reveals diamond-like shaped patterns due to the quantized Coulomb interaction (as predicted by the orthodox theory and observed in experiments). While the MCSCG treatment is able to cope with the mixture of many-body configurations, the Hartree theory only provides a mean interaction potential for the description of the Coulomb interaction.

In addition, Fig. 5 shows $I_{\rm D}(V_{\rm GS})$ curves for different drain voltages $V_{\rm DS}$. In the MCSCG case (Fig. 5 (b)), single-electron transport can be identified in terms of Coulomb oscillations for the two lowest $V_{\rm DS}$, whereas the Hartree-only simulation (Fig. 5(a)) lacks these features; the Hartree-only case exhibits broader peaks solely due to the single-particle levels of the system. However, with increasing $V_{\rm DS}$, both approaches become equivalent. (Note that the sub-threshold regime shows the regular behavior and has been omitted here.)

Finally, Fig. 6 shows the room temperature ($T = 300$K) characteristics. Apart from the slight modulation in the MCSCG calculation (Fig. 6(b)), which is a remnant of the Coulomb oscillation, the Hartree (Fig. 6(a)) and MCSCG (Fig. 5 (b)) results are in good agreement. Effects beyond a mean-field picture of the system will obviously have a significant impact on application-relevant device properties such as the system capacitance and the transconductance.

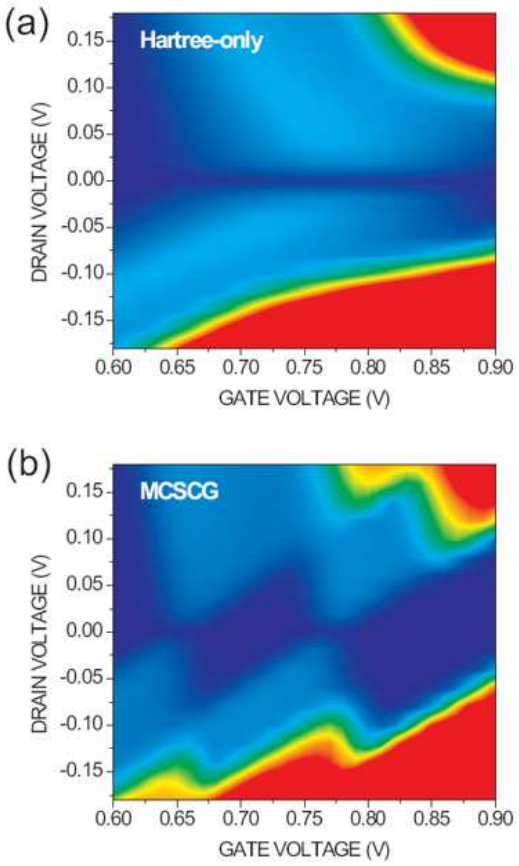

Fig. 4. (a) Color plot of the total drain current for the Hartree-only case at $T = 77$K (blue = 0nA, red = 5nA). (b) Color plot of the total drain current for the MCSCG case at $T = 77$K. (blue = 0nA, red = 5nA).

IV. Conclusion

In summary, we have compared for the first time the conventional Hartree NEGF with the MCSCG and have shown that the multi-configurational approach is able to describe single-electron charging effects in the low temperature limit for a realistic FET structure. In case of strong nonequilibrium (with an almost depleted channel) and room temperature conditions, the MCSCG and the well-established Hartree approximation lead to equivalent results for the discussed example of a nanowire MOSFET. As such, the MCSCG yields a seamless transition from the single-electron transport regime to transistor operation at room temperature. For realistic FETs with a large number of sites where a full Fock space formulation becomes impossible, the MCSCG permits a selfconsistent Fock space treatment of states which are responsible for few-electron charging effects.

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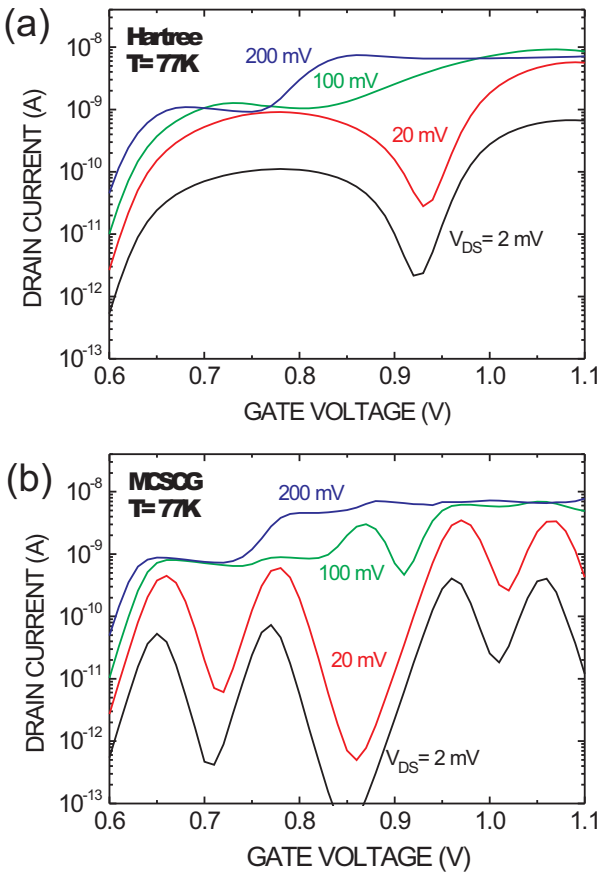

Fig. 5. (a) Transfer characteristics, Hartree-only at $T = 77$K. (b) Transfer characteristics, MCSCG approach at $T = 77$K.

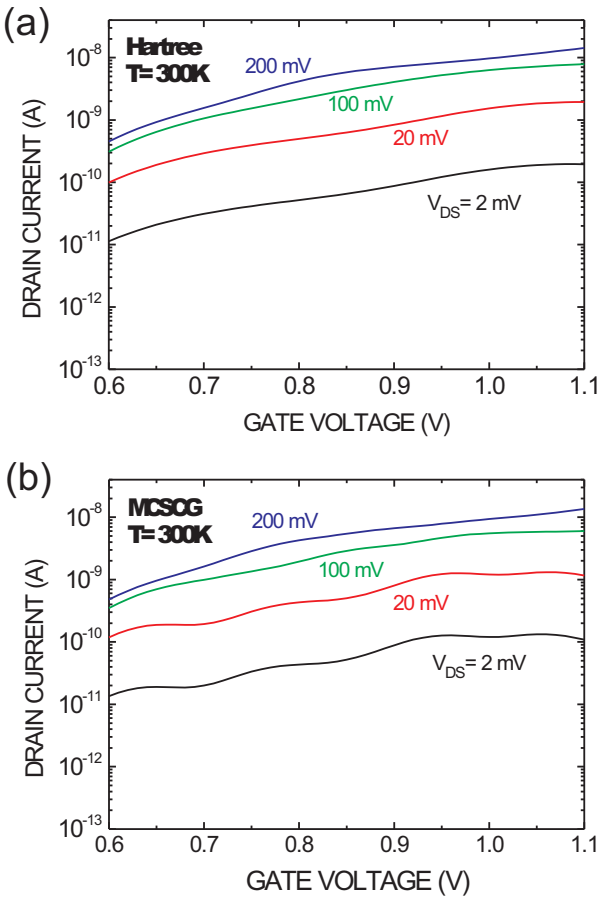

Fig. 6. (a) Transfer characteristics, Hartree-only at $T = 300$K. (b) Transfer characteristics, MCSCG approach at $T = 300$K.

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